

(19) World Intellectual Property Organization
International Bureau



(43) International Publication Date
29 September 2005 (29.09.2005)

PCT

(10) International Publication Number
WO 2005/091178 A3

(51) International Patent Classification:
G06F 19/00 (2006.01)

(21) International Application Number:
PCT/EP2005/050778

(22) International Filing Date:
24 February 2005 (24.02.2005)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
04290701.4 15 March 2004 (15.03.2004) EP

(71) Applicant (for all designated States except US): **AVANT-GARDE MATERIALS SIMULATION SARL** [FR/FR]; 30bis, rue du Vieil Abreuvoir, F-78100 St-Germain-en-Laye (FR).

(72) Inventor; and

(75) Inventor/Applicant (for US only): **NEUMANN, Marcus, A.** [DE/FR]; 30bis, rue du Vieil Abreuvoir, F-78100 St-Germain-en-Laye (FR).

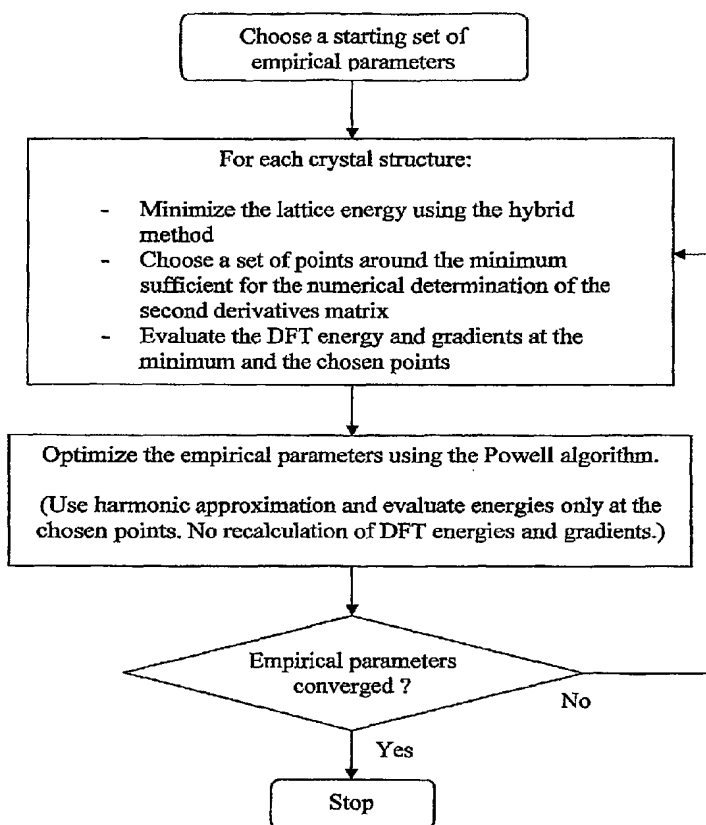
(74) Agent: **BETTEN & RESCH**; Theatinerstr. 8, 80333 Munich (DE).

(81) Designated States (unless otherwise indicated, for every kind of national protection available): AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW.

(84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

[Continued on next page]

(54) Title: METHOD FOR ENERGY RANKING OF MOLECULAR CRYSTALS USING DFT CALCULATIONS AND EMPIRICAL VAN DER WAALS POTENTIALS



(57) Abstract: The invention refers to a method for the accurate determination of van der Waals parameters for high-precision determination of crystal structures and/or energies, comprising the steps of: numerically simulating at least one crystal structure based on density functional theory (DFT) calculations combined with a potential energy term representing van der Waals interactions; providing reference data containing accurate information about said at least one crystal structure; defining a deviation function (F) quantifying a deviation between said reference data and said at least one simulated crystal structure; fitting at least one parameter of said van der Waals potential term in such a way as to minimize said deviation function (F); and obtaining the accurate van der Waals parameters from the best fit. The invention furthermore deals with a hybrid method for the accurate van der Waals parameters from the best fit. The invention furthermore deals with a hybrid method for the accurate determination of crystal structures and/or energies based on such a parameter determination as well as the general application of such a hybrid method to the energy ranking of polymorphic crystal structures.

WO 2005/091178 A3



Published:

- with international search report
- before the expiration of the time limit for amending the claims and to be republished in the event of receipt of amendments

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

(88) Date of publication of the international search report:

20 April 2006